Supporting Information for

Antiparallel double-stranded BODIPY–porphyrin dyad assembled by a self-complementary B–F···Zn interaction

Mitsuhiko Morisue,[a] Shinya Nakano,[a] Masaki Shimizu,[a] and Takashi Yumura[b]

[a]Faculty of Molecular Chemistry and Engineering, and [b]Faculty of Materials Science and Engineering, Kyoto Institute of Technology, Matsugasaki, Sakyo-ku, Kyoto 606-8585, Japan.

1. General Method

NMR spectra were recorded on Bruker AVANCE II 300 and AVANCE III 600. Tetramethylsilane (TMS) was used as the internal standard for ^{1}H NMR spectra, and hexafluorobenzene (δ = 164.9 ppm) was used as the internal standard for ^{19}F NMR spectra. Matrix-assisted laser-dissociation ionization time-of-flight (MALDI–TOF) mass spectra were recorded on mass spectrometer (Bruker, Autoflex Speed). UV/vis absorption spectra were recorded on a spectrophotometer (Shimadzu, UV-1800) equipped with a Peltier thermoelectric temperature controlling unit (Shimadzu, TCC-240A). Chloroform, spectral grade containing amylene as the stabilizer, was used as purchased from Kanto Chemical Co., Inc.

2. ^{1}H DOSY measurements.

Diffusion ordered NMR spectra (Figure S1) were recorded on JNM-ECA600 (JEOL). The result was performed with calibration by using residual H_2O in D_2O. The diffusion constant of $(\mathbf{1})_2$ was determined as 4.3×10^{-10} m^2 s^{-1}, which was somewhat smaller than 3.9×10^{-10} m^2 s^{-1} of **1**·Py. Although the axially coordinating pyridine should unambiguously increases the hydrodynamic volume of **1**·Py, the hydrodynamic volume of $(\mathbf{1})_2$ was nearly comparable. The comparison suggested the compact structure of the conformationally rigid $(\mathbf{1})_2$.

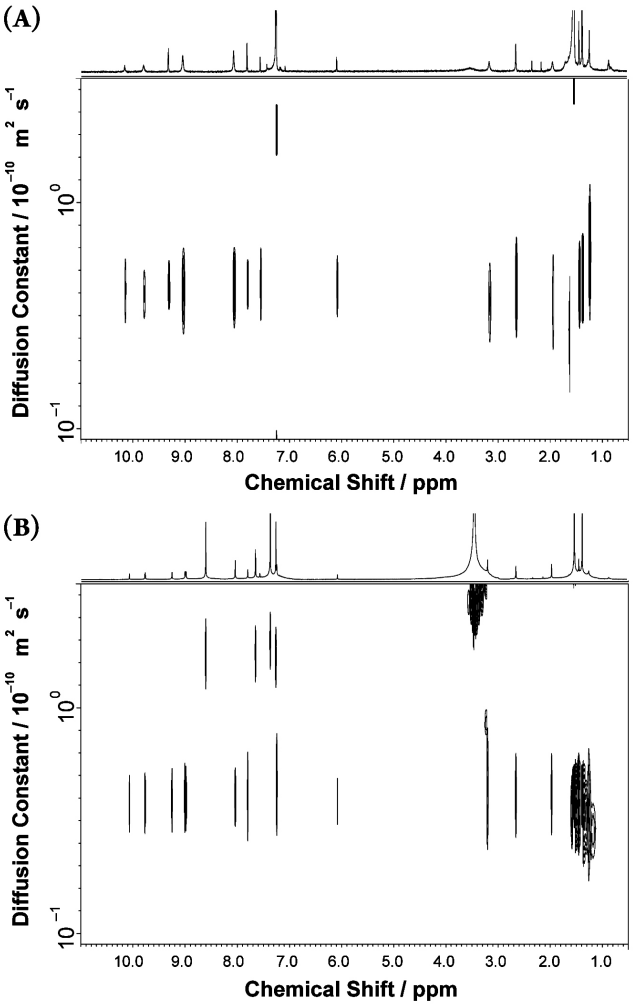


Fig. S1. DOSY spectra of $(\mathbf{1})_2$ ([**1**] = 5 × 10^{-4} M) at 292 K in $CDCl_3$ (A) and **1**·Py ([**1**] = 6 × 10^{-4} M) at 292 K in $CDCl_3$ with 10% of pyridine-d_5 (B).

3. Microscopic binding of pyridine to zinc porphyrin.

It was difficult to directly estimate the microscopic binding constant, K_μ = [**1**·Py]/[**1**][Py], because **1** assembled into (**1**)$_2$ even in very dilute solution. Then, we employed a model zinc porphyrin **2** to estimate the K_μ value (Fig. S2). Based on the global fitting analysis of the titration isotherms gave $K_\mu = 1.83 \times 10^5$ M^{-1}. Porphyrin **2** was synthesized according to the reported procedures.[S1]

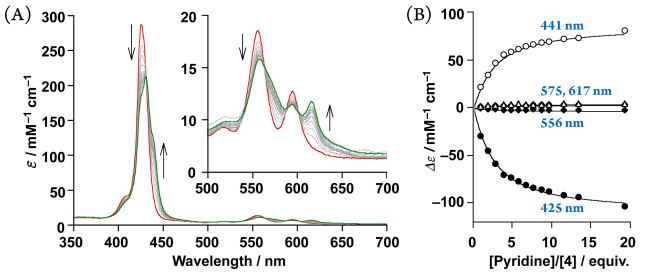
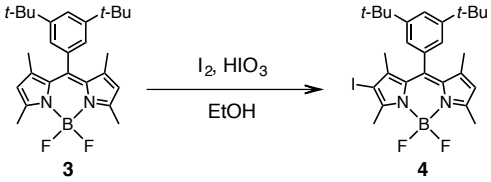


Fig. S2. Spectrometric titration of **2** with pyridine ([**2**]$_0$ = 2.58 × 10^{-6} M) at 298 K in $CHCl_3$ (A), and its global fitting analysts of titration isotherms assuming K_μ = [**2**·Py]/[**2**][Py] = 1.83 × 10^5 M^{-1} (B).

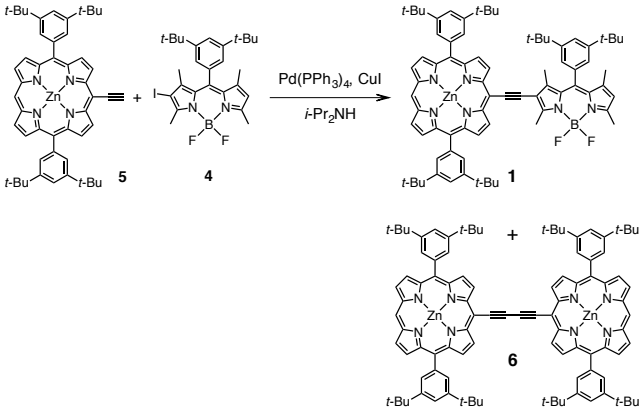
4. Synthesis

4.1. Synthesis of 4.



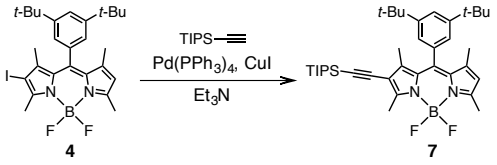
The precursor BODIPY **3** was prepared according to the reported procedures.[S2] A solution of **3** (0.15 g, 0.34 mmol) and iodic acid (24 mg, 0.14 mmol) in ethanol (8 mL) was added dropwise a solution of iodine (34 mg, 0.13 mmol) in ethanol (15 mL) at room temperature, and then the mixture was stirred at 60 °C for 2.5 h. To the reaction was added aqueous sodium thiosulfate, and the products were extracted with chloroform. The organic layer separated was dried over anhydrous sodium sulfate, and the crude product was subjected to silica gel chromatography with hexane/ethyl acetate (60/1). The product **4** was obtained as orange solid in a 55% yield (110 mg, 0.19 mmol). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.49 (t, J = 1.8 Hz, 1H; 4-Ar), 7.09 (d, ^3J = 1.8 Hz, 2H; 2,6-Ar), 6.04 (s, 1H, pyrrole-β), 2.64 (s, 3H; α-Me), 2.57 (s, 3H; α-Me), 1.36 (s, 6H; β-Me), 1.32 (s, 18 H; *t*-Bu) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ 157.4, 154.1, 152.2, 145.2, 143.2, 143.0, 133.8, 131.9, 131.0, 122.0, 84.1, 35.1, 31.4, 16.4, 15.7, 14.7, 14.3 ppm. MALDI-TOF MS (dithranol): m/z calc for $C_{27}H_{34}BF_2IN_2$: 562.18; found 561.246 [M]$^+$.

4.2. Synthesis of 1.



The precursor porphyrin **5** was prepared according to the reported procedures.[S3] A solution of **5** (0.11 g, 0.14 mmol), **4** (92 mg, 0.16 mmol), $Pd(PPh_3)_2Cl_2$ (7.3 mg, 10 μmol) in diisopropylamine (7 mL) and toluene (5 mL) was degassed via freeze-pump-thaw cycles before addition of CuI (7.4 mg, 39 μmol). The mixture was stirred at 50 °C under Ar atmosphere for 15 h. The reaction mixture was diluted with excess toluene, and washed with water. The organic layer separated was dried over anhydrous magnesium sulfate. The crude material was passed through silica plug with toluene/ethyl acetate (3/1, v/v). Then, the BODIPY–porphyrin dyad **1** and porphyrin dimer **6** were eluted by size-exclusion chromatography with 5% pyridine in toluene. The product **1** was obtained as dark green solid in a 61% yield (0.10 g, 84 μmol), and the product **3** was obtained as dark green solid in a 16% yield (35 mg, 22 μmol). **1**: ^{1}H NMR (300 MHz, THF-d_8): δ 10.17 (s, 1H; porphyrin-*meso*), 9.78 (d, ^3J = 4.5 Hz, 2H; porphyrin-β), 9.32 (d, ^3J = 4.5 Hz, 2H; porphyrin-β), 8.96 (d, J = 4.8 Hz, 4H; porphyrin-β), 8.14 (d, ^3J = 1.2 Hz, 4H; Ar), 7.95 (s, 2H; Ar), 7.72 (s, 1H; Ar), 7.45 (d, J = 1.8 Hz, 2H; Ar), 6.21 (s, 1H; BODIPY-β), 3.18 (s, 3H; BODIPY α-Me), 2.65 (s, 3H; BODIPY α-Me), 2.05 (s, 3H; BODIPY β-Me), 1.55 (s, 3H; BODIPY β-Me). ^{13}C NMR (75 MHz, THF-d_8): δ 152.4 ppm. MALDI-TOF MS (dithranol): m/z calc for $C_{77}H_{85}BF_2N_6Zn$: 1206.62; found 1205.2 [M]$^+$. **6**: ^{1}H NMR (300 MHz, $CDCl_3$): δ 10.18 (s, 2H; porphyrin-*meso*), 10.05 (d, ^3J = 4.5 Hz, 4H; porphyrin-β), 9.33 (d, ^3J = 4.5 Hz, 4H; porphyrin-β), 9.18 (d, ^3J = 4.5 Hz, 4H; porphyrin-β), 9.08 (d, ^3J = 4.5 Hz, 4H; porphyrin-β), 8.14 (d, ^3J = 4.5 Hz, 4H; Ar), 7.85 (s, 2H; Ar), 1.59 (s, 36H; *t*-Bu) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ 153.0, 151.1, 150.1, 149.5, 148.8, 141.4, 133.6, 132.8, 130.0, 123.3, 121.0 35.1, 31.8 ppm. MALDI-TOF MS (dithranol): m/z calc for $C_{100}H_{102}N_8Zn_2$: 1542.68; found 1543.04 [M]$^+$.

4.3. Synthesis of 8.



A solution of **5** (56 mg, 0.1 mmol), $Pd(PPh_3)_4$ (1.5 mg, 1.3 μmol), CuI (2.9 mg, 15 μmol) in triethylemine (7 mL) was degassed by repetitive freeze-pump-thaw cycles before addition of triisopropylsilylacetylene (75 μL, 0.31 mmol). The mixture was stirred at 50 °C under Ar atmosphere for 15 h. The reaction mixture diluted with toluene was washed with water, and the organic layer separated was dried over anhydrous magnesium sulfate. The product **8** was isolated by silica gel column chromatography with toluene as the eluent and subsequent size-exclusion chromatography with toluene/pyridine (95:5). The product 8 was obtained as orange solid in 82% yield (50 mg, 82 μmol). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.49 (s, 1H; Ar), 7.08 (d, ^3J = 1.5 Hz, 2H; Ar), 6.02 (s, 1H; BODIPY-β), 2.65 (s, 3H; α-Me), 2.57 (s, 3H; α-Me), 1.45 (s, 3H; α-Me), 1.37 (s, 3H; α-Me), 1.01 (s, 3H; *t*-Bu) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ 157.1, 156.8, 152.1, 144.6, 143.7, 143.4, 133.7, 132.5, 130.2, 122.1, 121.9, 121.8, 115.6, 99.4, 97.0, 90.2, 81.6, 35.1, 31.4, 18.7, 18.6, 14.7, 14.2, 13.4, 13.0, 11.3 ppm. ^{19}F NMR (282 Hz, $CDCl_3$): δ –149.5 (dd, $J_{19F-19F}$ = 65.1 Hz, $J_{11B-19F}$ = 25.4 Hz) ppm. MALDI-TOF MS (dithranol): m/z calc for $C_{38}H_{55}BF_2N_2Si$: 616.42; found 615.5 $[M]^+$.

5. Computational Investigations

To investigate interactions of $(\mathbf{1})_2$, density functional theory (DFT) calculations were performed by using dispersion-corrected B97 functional (B97D). We constructed initial structures for BODIPY-porphyrin dyad $(\mathbf{1})_2$. Then, structure for $(\mathbf{1})_2$ was fully optimized. During the DFT optimization implemented in the Gaussian 09 code, we used the 6-311G* basis set for the Zn atoms, and the 6-31G* basis set for the other atoms. After obtaining the optimized structure for $(\mathbf{1})_2$, the interaction energy (E_{bind}) was evaluated in the following equation.

$$E_{bind} = E_{total}((\mathbf{1})_2) - 2 \times E_{total}(\mathbf{1}) \qquad \text{(S1)}$$

where $E_{total}((\mathbf{1})_2)$ and $E_{total}(\mathbf{1})$ are the total energies of the optimized structures for $(\mathbf{1})_2$ and **1**, respectively. The optimized structures for $(\mathbf{1})_2$ and **1** are displayed in Fig. 2 and Fig S3, respectively. In estimating the E_{bind} values in $(\mathbf{1})_2$, basis set superposition errors (BSSEs) were corrected.

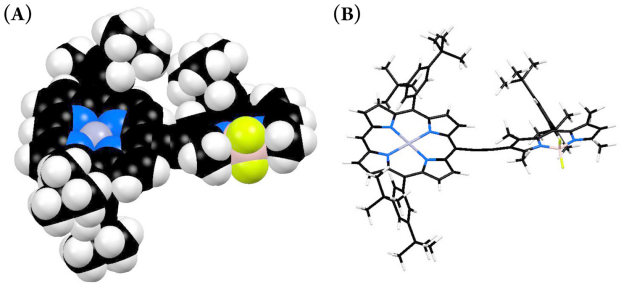


Fig. S3. B97D-optimized structures for **1** as a space-filling model (A) and stick image (B).

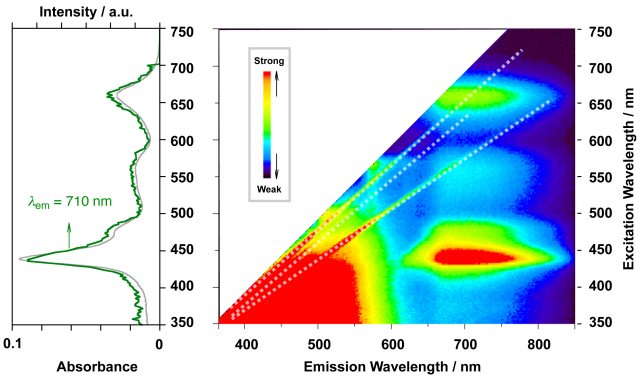


Fig. S4. Excitation spectrum of **1** monitored at 710 nm (green line) together with absorption spectrum (grey line) (left panel), and emission–excitation contour map of **1** in pyridine, where white dotted lines indicate Raman scattering of pyridine (right panel).

References

[S1] Y. Liu, H. Lin, J. T. Dy, K. Tamaki, J. Nakazaki, D. Nakayama, S. Uchida, T. Kubo, H. Segawa, *Chem. Commun.* 2011, **47**, 4010–4012.

[S2] T. Ozdemir, S. Atilgan, I. Kutuk, L. T. Yildirim, A. Tulek, M. Bayindir, E. U. Akkaya, *Org. Lett.* 2009, **11**, 2105–2107.

[S3] T. E. O. Screen, I. M. Blake, L. H. Rees, W. Clegg, S. J. Borwick, H. L. Anderson, *J. Chem. Soc. Perkin Trans. 1*, 2002, 320–329.

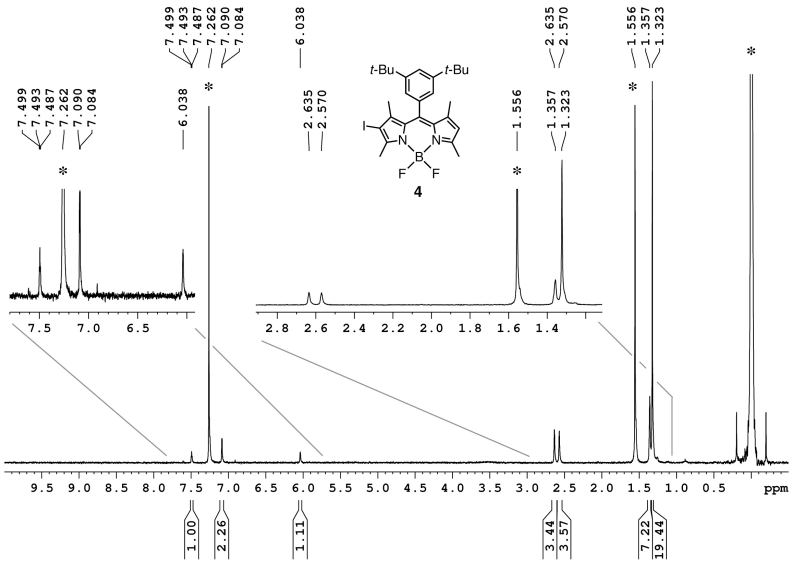


Fig. S5. ^{1}H NMR spectrum of **4** in $CDCl_3$ (300 MHz). Asterisk indicates residual solvent and water.

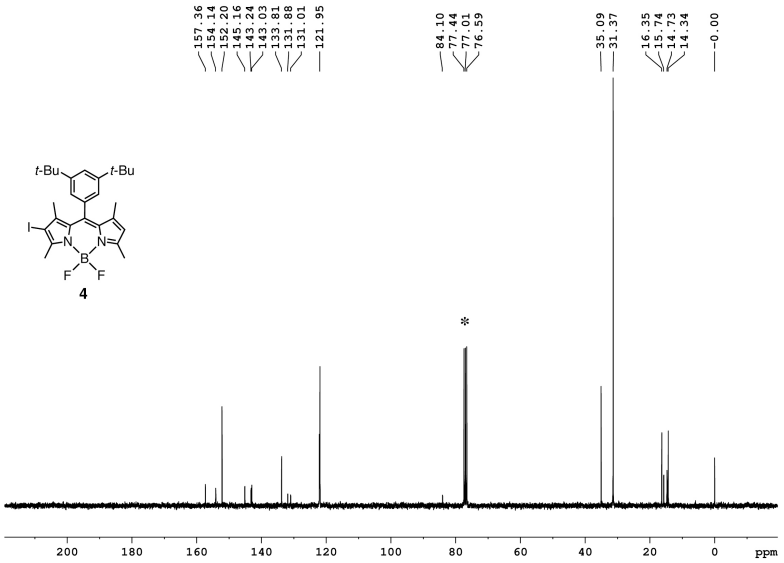


Fig. S6. ^{13}C NMR spectrum of **4** in $CDCl_3$ (75 MHz). Asterisk indicates solvent.

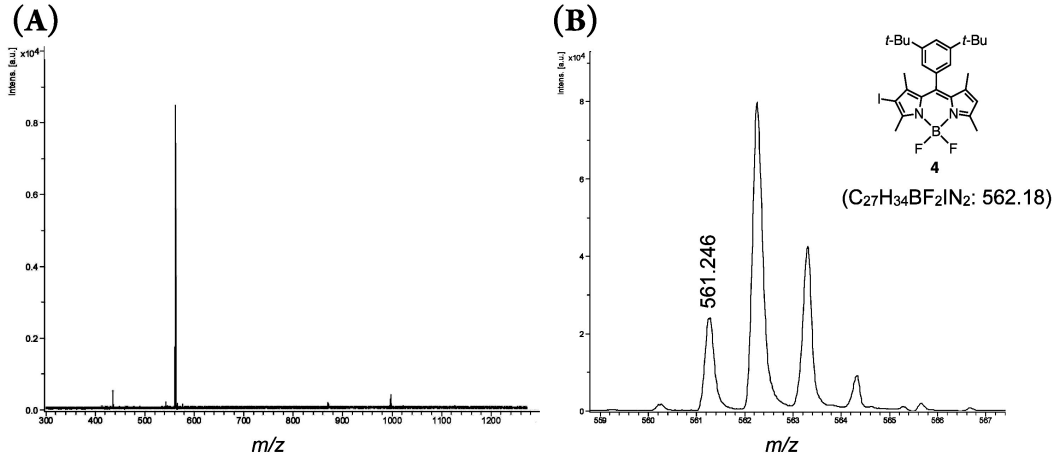


Fig. S7. MALDI TOF MS spectrum of **4**. Spectrum B magnifies the isotopic pattern obtained in A.

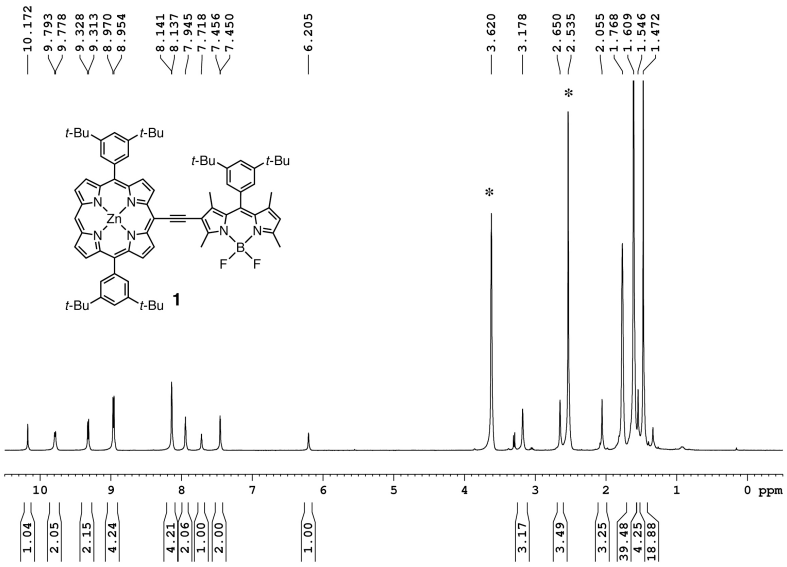


Fig. S8. ^{1}H NMR spectrum of **1** in THF-d_8 (300 MHz). Asterisk indicates residual solvent.

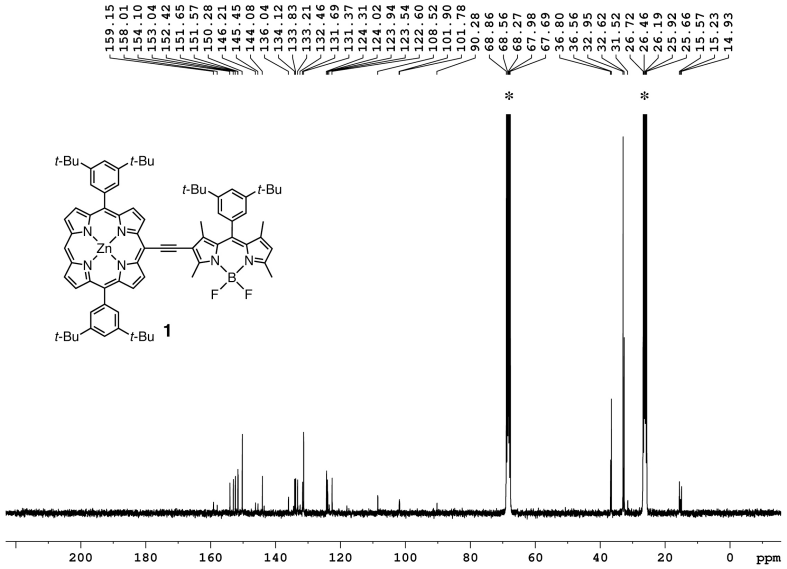


Fig. S9. ^{13}C NMR spectrum of **1** in THF-d_8 (75 MHz). Asterisk indicates solvent.

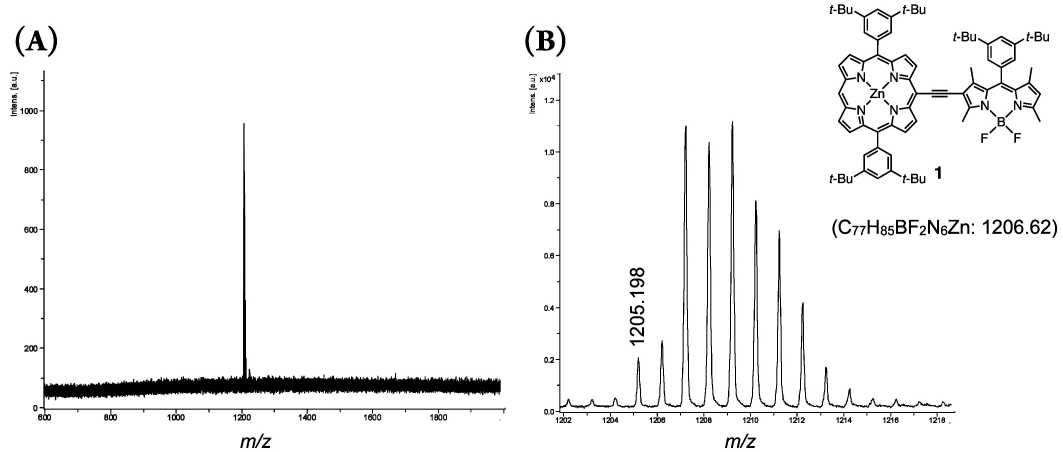


Fig. S10. MALDI TOF MS spectrum of **1**. Spectrum B magnifies the isotopic pattern.

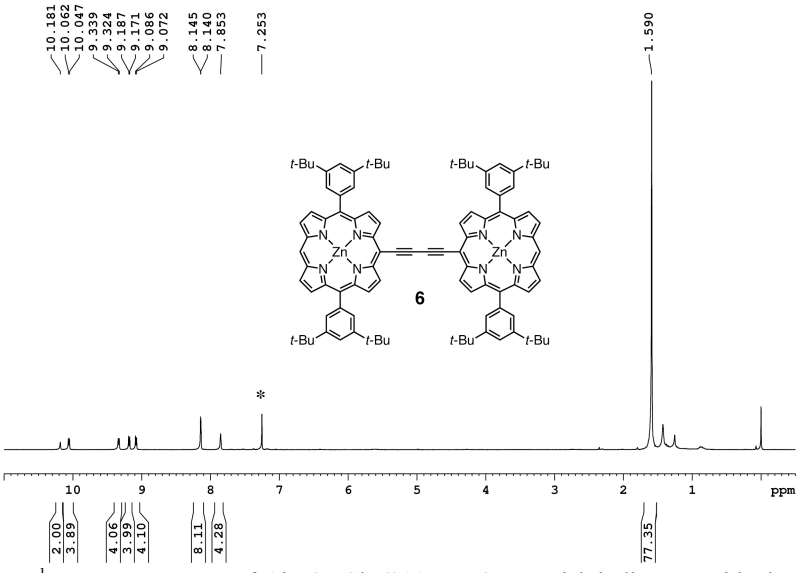


Fig. S11. ^{1}H NMR spectrum of **6** in $CDCl_3$ (300 MHz). Asterisk indicates residual solvent.

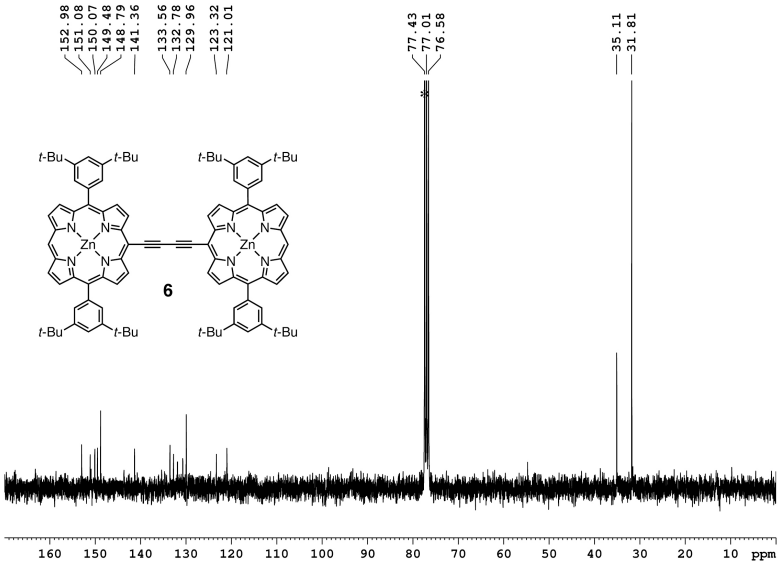


Fig. S12. ^{13}C NMR spectrum of **6** in $CDCl_3$ (75 MHz). Asterisk indicates solvent.

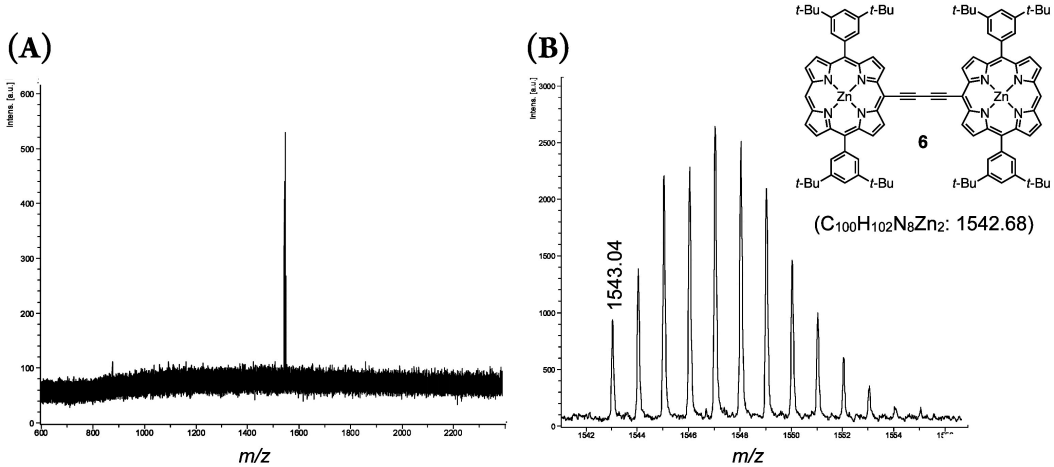


Fig. S13. MALDI TOF MS spectrum of **6**.

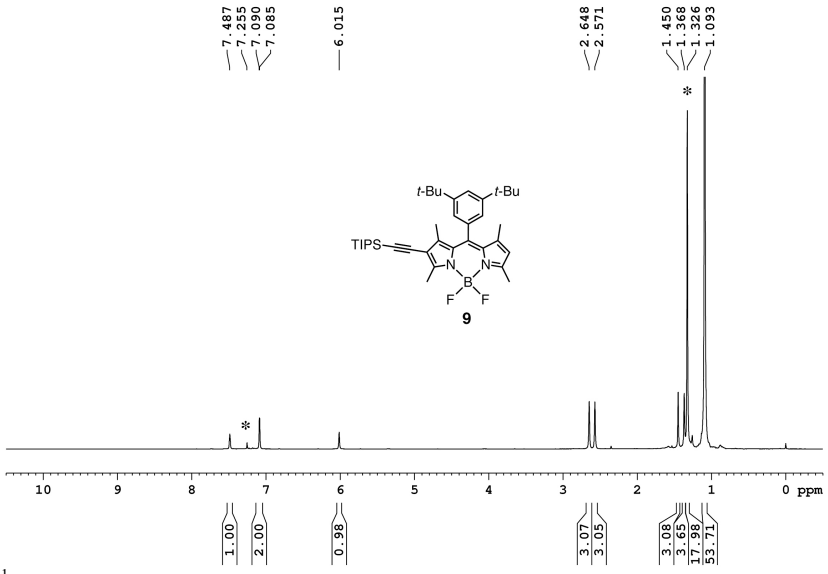


Fig. S14. ^{1}H NMR spectrum of **9** in $CDCl_3$ (300 MHz). Asterisk indicates residual solvent and water.

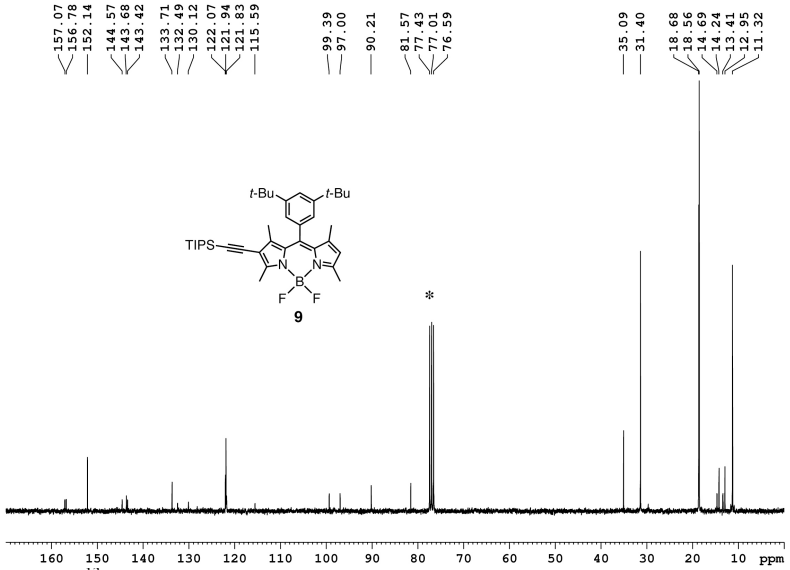


Fig. S15. ^{13}C NMR spectrum of **9** in $CDCl_3$ (75 MHz). Asterisk indicates solvent.

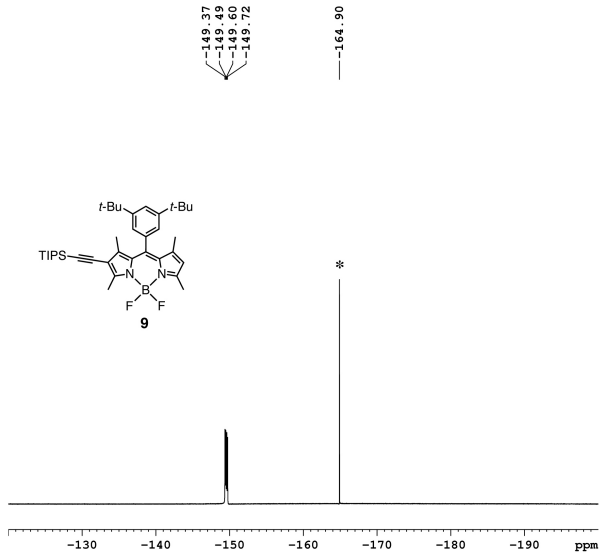


Fig. S16. ^{19}F NMR spectrum of **9** in $CDCl_3$ (282 MHz). Asterisk indicates hexafluorobenzene as the internal standard.

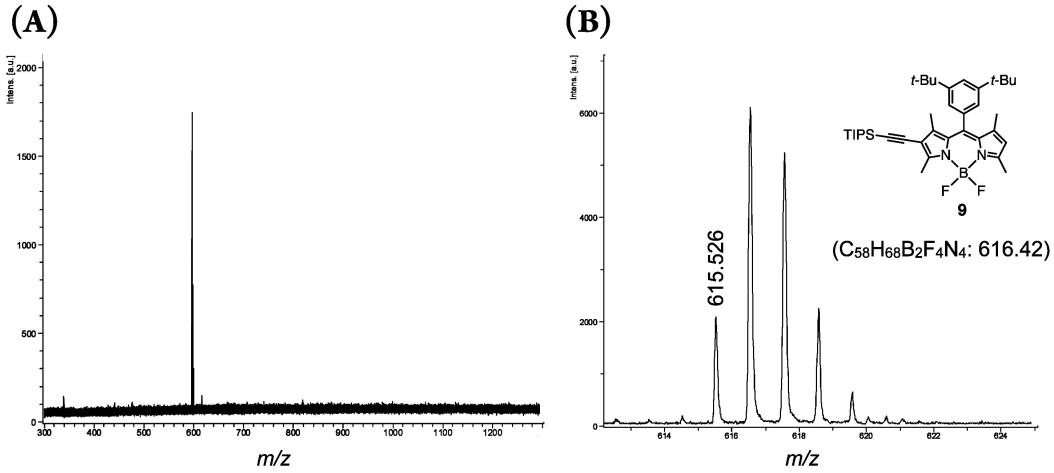


Fig. S17. MALDI TOD MS spectrum of **9**.

6. Cartesian coordinates in optimized structures obtained from B97-D calculations

6.1. C_i–$(1)_2$ for Fig. 2A and Fig S18.

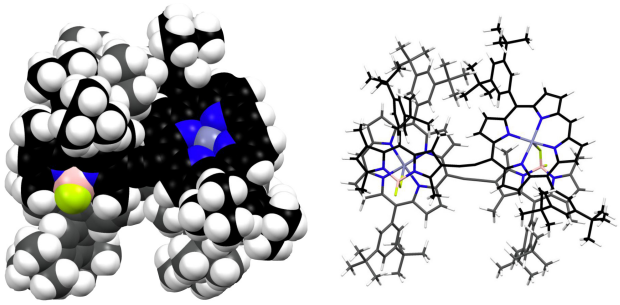


Fig. S18. B97D-optimized structures for C_i–$(\mathbf{1})_2$ including 3,5-di-*tert*-butylphenyl groups.

C	-4.13258700	4.60399800	1.69782000
C	-2.87493100	5.29946900	1.91567900
C	-1.89424900	4.34346100	1.95528700
C	-2.55326400	3.07267800	1.75455100
N	-3.90488600	3.24613700	1.61213000
C	-5.38419500	5.24182700	1.52590800
C	-1.88711200	1.82180900	1.68676100
C	-2.52115500	0.56417900	1.46828100
C	-1.87099200	-0.69773500	1.70353700
C	-2.78437600	-1.67029900	1.40566400
C	-3.98820900	-0.99891700	0.95634300
N	-3.80702800	0.37404500	1.02955900
C	-5.17177500	-1.66059800	0.54775600
C	-6.38947000	-0.98911600	0.25825700
C	-7.62636900	-1.63563000	-0.13738200
C	-8.56590200	-0.64922100	-0.28790500
C	-7.91244200	0.59476400	0.03683900
N	-6.58590100	0.37384300	0.33623000
C	-8.57326700	1.82702400	0.11722500
C	-8.03740300	3.04749500	0.54534300
C	-8.77576200	4.28722900	0.63894400
C	-7.88169700	5.24739500	1.03604100
C	-6.59221500	4.58990000	1.17666500
N	-6.72356100	3.24873200	0.89652100
Zn	-5.22291700	1.85247200	0.82967900
C	-5.13675300	-3.15806000	0.52447800
C	-5.42285200	6.72831000	1.65844600
C	-0.47683500	1.77958300	1.82390100
C	0.73541600	1.57485800	1.84063200
F	4.94570000	-1.93047400	2.51599200

C	2.09102100	-0.91230700	3.17724300	C	-4.11736500	-3.85269800	-0.16501200
C	2.76331000	0.22297400	2.47748600	C	1.91507600	-3.81896500	1.20557400
C	2.12379200	1.35824800	1.88419600	C	0.51229200	-3.54812700	0.96979000
C	3.13104900	2.19752800	1.36161400	C	0.44374500	-2.40746800	0.21874900
C	4.37027400	1.57711900	1.69383900	C	1.80156800	-1.98297500	-0.01534600
N	4.09746600	0.35850100	2.34566800	N	2.68234600	-2.85058600	0.58336800
C	5.69846700	2.00347100	1.49616000	C	2.40148800	-4.92522500	1.94798100
C	6.78547600	1.18649000	1.86100800	C	2.14731200	-0.80889900	-0.74764400
C	8.19884300	1.42736800	1.85561800	C	3.47034000	-0.37693200	-1.02283600
C	8.78967400	0.25849100	2.34938100	C	3.79631300	0.81168900	-1.77192500
C	7.76306300	-0.65159400	2.68942000	C	5.16041800	0.82996300	-1.90119600
N	6.56213400	-0.09427500	2.39037100	C	5.66671400	-0.36070100	-1.24106700
C	7.87790400	-1.98149300	3.36143500	N	4.61407900	-1.05911900	-0.68293400
F	5.17236000	-0.54801200	4.33437000	C	7.02488000	-0.77006100	-1.23047700
B	5.18982800	-0.58883900	2.94112200	C	7.50985800	-1.95268400	-0.61216900
C	5.93428900	3.37598000	0.97884800	C	8.88067200	-2.43615700	-0.68660000
C	8.93566600	2.68008500	1.47269400	C	8.93147000	-3.60532800	0.02468300
C	2.85916400	3.42665500	0.54587900	C	7.59399600	-3.85566200	0.50904800
C	5.53388100	4.46851500	1.76862800	N	6.74726400	-2.84263200	0.11224300
C	5.72284300	5.78560300	1.32066300	C	7.23226800	-4.96362000	1.28682100
C	6.33055400	5.96645700	0.06434200	C	5.94992600	-5.29628300	1.74493100
C	6.74930100	4.89416100	-0.74592300	C	5.65039500	-6.40472300	2.62703000
C	6.54241400	3.58790900	-0.26914700	C	4.29625300	-6.38311100	2.83651400
C	-5.07506700	7.35567600	2.86370200	C	3.76986400	-5.27338400	2.05681400
C	-5.09281500	8.75985600	2.99115200	N	4.79887500	-4.61972100	1.41981500
C	-5.47750300	9.51583700	1.87222300	Zn	4.72857000	-2.77092000	0.46869600
C	-5.83348200	8.91873600	0.64174000	C	8.00719000	0.03204400	-2.02134600
C	-5.79724100	7.52067900	0.55172100	C	1.38196200	-5.80487900	2.59406300
C	-6.06947100	-3.90091400	1.27820900	C	1.03465600	-0.09751300	-1.28073400
C	-6.00480700	-5.30289200	1.34367500	C	-0.08903000	0.27700000	-1.61482600
C	-4.94593600	-5.94881600	0.67835800	F	-4.64339100	3.24597200	-1.04993800
C	-3.97714000	-5.24982900	-0.06511400	C	-1.61186100	3.07677200	-1.50181100

C	-2.14828600	1.73683900	-1.88136000	H	-2.76711000	6.37445000	2.01095500
C	-1.42930700	0.51219100	-1.98903900	H	-0.82429500	4.46885000	2.09260100
C	-2.33325600	-0.47522800	-2.46012200	H	-0.85914400	-0.81444700	2.06908800
C	-3.59267700	0.17521400	-2.61833500	H	-2.65780500	-2.73969400	1.50791500
N	-3.43138100	1.52027400	-2.24158300	H	-7.75799800	-2.69985400	-0.26514300
C	-4.85755300	-0.30431900	-3.04878200	H	-9.61243600	-0.75133300	-0.56397900
C	-5.98977400	0.54030100	-3.04678200	H	-9.62943500	1.82732100	-0.15392000
C	-7.34657300	0.35057500	-3.49319800	H	-9.83643200	4.39978300	0.42792300
C	-7.98764900	1.57906500	-3.31844100	H	-8.06529800	6.29946600	1.22533100
C	-7.05684100	2.50448700	-2.80059200	H	1.66454100	-0.56071700	4.13081000
N	-5.86726600	1.87687000	-2.62912500	H	2.78332500	-1.73455600	3.37101100
C	-7.23379100	3.96611400	-2.53688900	H	1.26364100	-1.28331900	2.55701000
F	-4.23386100	3.56334100	-3.29354100	H	9.85286200	0.08026100	2.48509100
B	-4.53377700	2.61184000	-2.31461000	H	7.27042900	-2.73140500	2.84372000
C	-4.95451200	-1.67062100	-3.63537300	H	7.49473900	-1.90744800	4.39142500
C	-8.01746300	-0.86563400	-4.06678600	H	8.92476800	-2.30849700	3.38400900
C	-1.95102100	-1.89811000	-2.72715500	H	8.41529700	3.57981900	1.82677300
C	-5.78962100	-2.66789100	-3.09077200	H	9.03514300	2.77609000	0.38143900
C	-5.92706800	-3.91025700	-3.73075800	H	9.94504900	2.66132700	1.90757100
C	-5.15054100	-4.15388300	-4.88526300	H	2.91291600	4.34698500	1.14833500
C	-4.29282400	-3.19051800	-5.43910800	H	1.84662300	3.35581800	0.12316400
C	-4.22433600	-1.93674700	-4.80414400	H	3.58764400	3.53197500	-0.26797500
C	1.33984300	-7.18314600	2.30918500	H	6.48391800	6.98300900	-0.29804000
C	0.34061900	-8.01517000	2.84468100	H	-4.78797200	6.73273200	3.71041100
C	-0.64916800	-7.42768300	3.65610200	H	-5.50233600	10.60166700	1.94385700
C	-0.65208400	-6.05037900	3.95115100	H	-6.04762900	7.01324400	-0.37725500
C	0.39154600	-5.26262400	3.43681500	H	-6.83465100	-3.35711500	1.82643000
C	9.20647400	0.50045500	-1.43854000	H	-4.85740300	-7.03147100	0.76536700
C	10.18933000	1.13718700	-2.21285600	H	-3.39990500	-3.26806600	-0.73079500
C	9.91548800	1.36837500	-3.57896100	H	-0.31428200	-4.15605800	1.30996000
C	8.72272000	0.94597900	-4.18647700	H	-0.44328300	-1.88957800	-0.11580200
C	7.78868300	0.25546600	-3.39118300	H	3.06673000	1.52328100	-2.14626200

H	5.76722000	1.56979000	-2.40834000
H	9.68750700	-1.95297800	-1.22494700
H	9.78652300	-4.25649900	0.18933400
H	8.04148600	-5.63573400	1.57547900
H	6.38529500	-7.09200300	3.03920600
H	3.70256000	-7.04397600	3.45897000
H	-0.61941700	2.95796400	-1.05038200
H	-2.28170600	3.57965300	-0.79661900
H	-1.53772400	3.71636600	-2.39587200
H	-9.02700200	1.79748900	-3.54768400
H	-6.67243500	4.54789700	-3.28456100
H	-6.83083400	4.23088200	-1.55280400
H	-8.29551400	4.23660100	-2.58254300
H	-8.24732700	-1.60368400	-3.28405800
H	-7.38855800	-1.37211600	-4.81108000
H	-8.96378800	-0.56856700	-4.54220300
H	-2.78324000	-2.58556000	-2.55587500
H	-1.09935000	-2.18493700	-2.09850400
H	-1.64274300	-2.03676900	-3.77485100
H	-6.35137000	-2.43027200	-2.19239000
H	-5.24691500	-5.12239000	-5.37197300
H	-3.58976200	-1.15074300	-5.21186200
H	2.09306600	-7.59683500	1.63954800
H	-1.44437500	-8.05209700	4.05326600
H	0.42513900	-4.19566700	3.65283900
H	9.35574000	0.31923700	-0.37724000
H	10.65697600	1.89562300	-4.17463100
H	6.87693200	-0.13577800	-3.84030400
C	-3.45738500	-3.43722000	-6.70736300
C	-3.89935300	-2.43811500	-7.80719200
C	-1.95735300	-3.21104900	-6.38821800
C	-6.94758500	-4.98096800	-3.29747000
C	-7.72339800	-4.58656700	-2.02819500
C	-6.23926300	-6.32326200	-3.00339500
C	-7.96919100	-5.17341900	-4.44973100
C	-4.69194700	9.39398400	4.33519000
C	-4.76306600	10.93501500	4.30896800
C	-5.64271000	8.88243500	5.44788200
C	-3.23704500	8.97985400	4.67750400
C	-6.23250000	9.81571000	-0.54369400
C	-6.59236900	9.00231200	-1.80561600
C	-7.46590800	10.66786800	-0.14810700
C	-5.05251200	10.75836200	-0.89314500
C	-2.74922300	-6.01245800	-0.60634000
C	-1.82841200	-5.12092100	-1.46214400
C	-3.14788700	-7.23581800	-1.46910100
C	-1.95224200	-6.52909500	0.61991400
C	-7.01750500	-6.14746900	2.13574400
C	-8.13087600	-5.29025700	2.77361700
C	-6.27627400	-6.90727000	3.26589100
C	-7.68230500	-7.17086100	1.17938500
C	0.35038600	-9.51512800	2.49621400
C	0.21548000	-9.69042200	0.96136300
C	1.69276100	-10.13464600	2.96372100
C	-1.77173600	-5.37232500	4.76332800
C	-1.16089100	-4.64206500	5.98592800
C	-2.48882000	-4.33510900	3.85788400
C	-2.82737800	-6.37617400	5.27263200
C	11.53543500	1.59879600	-1.62290800
C	12.70436800	1.12671900	-2.52658300
C	11.54682200	3.14681500	-1.54808000
C	11.78404000	1.02381400	-0.21128400
C	8.42231000	1.15521100	-5.68181600
C	8.38004200	-0.23070600	-6.37663100

C	7.04637600	1.84846600	-5.85552900	H	-2.54073400	9.34375800	3.90656500
C	9.48822000	2.02277900	-6.38393700	H	-3.13724500	7.88681900	4.74113000
C	5.27595700	7.01467200	2.13042500	H	-2.94099400	9.41053900	5.64709000
C	6.50543500	7.91068200	2.42755400	H	-7.44058000	8.32688900	-1.61688300
C	4.24414200	7.82008300	1.29852700	H	-5.73935200	8.39826000	-2.14896500
C	4.61947600	6.62934400	3.47320800	H	-6.87445900	9.69089700	-2.61585300
C	7.41544600	5.19248400	-2.09917900	H	-8.32183200	10.01952800	0.09335000
C	6.43606600	6.00131300	-2.98722700	H	-7.75118900	11.32751500	-0.98282600
C	8.70124400	6.02503500	-1.85879300	H	-7.25304000	11.29575300	0.72894000
H	5.06176200	4.26517500	2.72725100	H	-4.16774600	10.17515500	-1.18949300
H	6.85280600	2.72066000	-0.84461800	H	-4.77710500	11.38806200	-0.03481000
H	-3.29937000	-2.59052400	-8.71817300	H	-5.33285600	11.41872200	-1.72903900
H	-3.76542900	-1.39820800	-7.47650800	H	-0.97024800	-5.71371200	-1.81138300
H	-4.96076500	-2.58454500	-8.05814800	H	-1.43305800	-4.27074400	-0.89247200
H	-1.35063500	-3.38544700	-7.29054300	H	-2.36591100	-4.73727100	-2.34115300
H	-1.61863700	-3.90114000	-5.60081000	H	-3.86228200	-7.89170800	-0.95094600
H	-1.77153900	-2.18218500	-6.04808700	H	-2.24595600	-7.82646700	-1.69312400
H	-8.44891200	-5.37761900	-1.78582100	H	-3.59474300	-6.91989100	-2.42083000
H	-7.04280000	-4.47285500	-1.17419000	H	-2.53275800	-7.27437900	1.18296600
H	-8.27890100	-3.64893100	-2.17358800	H	-1.70491700	-5.71925700	1.31634500
H	-5.63289100	-6.66510300	-3.85468500	H	-1.01263800	-6.99813500	0.29717000
H	-6.98904900	-7.09973000	-2.78354900	H	-8.68852800	-4.72917500	2.00849800
H	-5.59024100	-6.21414100	-2.12649900	H	-7.71901700	-4.57101700	3.49706500
H	-7.47517000	-5.50822100	-5.37316500	H	-8.83756400	-5.94456500	3.30534700
H	-8.49400900	-4.22992600	-4.66383000	H	-5.49795600	-7.56811600	2.85710600
H	-8.71461000	-5.93177400	-4.16245700	H	-6.98726400	-7.52480900	3.83707500
H	-5.78458000	11.28368300	4.09385100	H	-5.79358100	-6.19916500	3.95535400
H	-4.08607400	11.35349500	3.54879700	H	-6.93556600	-7.83768200	0.72486000
H	-4.46491000	11.33233600	5.29045500	H	-8.21362800	-6.65148900	0.36816100
H	-5.35377600	9.31524000	6.41873400	H	-8.40555900	-7.78988000	1.73349500
H	-5.60351100	7.78728600	5.53403200	H	1.02624100	-9.17396800	0.42800500
H	-6.68182300	9.17256700	5.23093100	H	-0.74250200	-9.28064700	0.60955200

H	0.25754700	-10.75958300	0.69936000
H	1.80539000	-10.03284400	4.05391200
H	2.54857600	-9.63918600	2.48311500
H	1.72498700	-11.20540100	2.70729800
H	-0.43423700	-3.87852200	5.67391900
H	-1.95608700	-4.14259100	6.56115800
H	-0.64572100	-5.35588400	6.64639100
H	-3.27161300	-3.80951600	4.42677400
H	-2.96355200	-4.82719600	2.99605400
H	-1.78345500	-3.58136300	3.48153000
H	-2.37582300	-7.13409700	5.93106100
H	-3.32459000	-6.89112100	4.43745900
H	-3.59595100	-5.83748000	5.84627600
H	12.64962900	1.56149200	-3.53428400
H	12.69883500	0.03069600	-2.62411800
H	13.66289700	1.43290900	-2.07945800
H	12.51487300	3.50474500	-1.16290900
H	10.75213500	3.50803200	-0.87923400
H	11.38146400	3.58799100	-2.54189200
H	11.76144600	-0.07637900	-0.22606700
H	11.03256600	1.37159500	0.50707500
H	12.77334300	1.34629100	0.14644300
H	6.81918400	1.95894000	-6.92733600
H	7.05387200	2.84582600	-5.39431600
H	6.23791300	1.26342600	-5.39467700
H	10.47856400	1.54382000	-6.35498500
H	9.56814500	3.01437700	-5.91246400
H	9.20936100	2.16391500	-7.43856700
H	6.99389000	8.24100600	1.49941000
H	7.24644000	7.36290600	3.02915700
H	6.19179600	8.80501300	2.98824200
H	3.91668700	8.70671000	1.86363700
H	3.36126500	7.20250500	1.07459500
H	4.67487300	8.15920500	0.34530900
H	5.31614500	6.06632300	4.11223600
H	3.71921200	6.01537500	3.31824600
H	4.32170500	7.54189300	4.01002700
H	6.15006200	6.95073300	-2.51165700
H	5.51938900	5.42183900	-3.17469300
H	6.90909000	6.23002100	-3.95523700
H	9.41534500	5.46130600	-1.24051300
H	8.47619700	6.97261700	-1.34822700
H	9.18341100	6.25754300	-2.82146600
H	7.60701300	-0.87185200	-5.92898700
H	9.34940200	-0.74223200	-6.27779700
H	8.15378900	-0.11022000	-7.44805000
C	-3.62198900	-4.87020400	-7.25570800
H	-4.66554700	-5.07342400	-7.54018400
H	-3.31170300	-5.62028400	-6.51240800
H	-2.99390400	-4.99297100	-8.15023600
C	7.80558100	3.90941000	-2.85380700
H	6.92265400	3.30244200	-3.09607800
H	8.49938900	3.28369600	-2.27946200
H	8.29992100	4.17486100	-3.79939800
C	-0.80204300	-10.28888300	3.17012100
H	-1.78157700	-9.90849900	2.84259200
H	-0.74889000	-10.21127800	4.26658100
H	-0.73861700	-11.35252100	2.89692100

6.2. C_2–$(1)_2$ for Fig. 2B and Fig. S19.

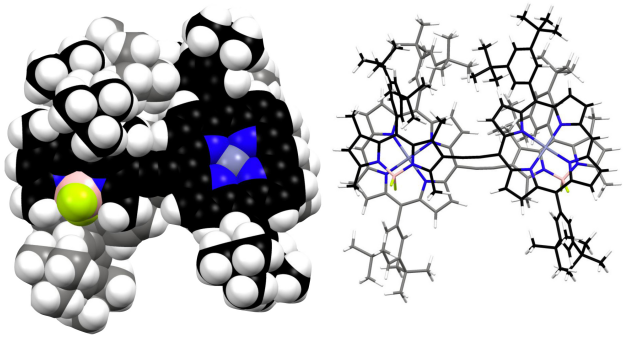


Fig. S19. B97D-optimized structures for C_2–$(\mathbf{1})_2$ including 3,5-di-*tert*-butylphenyl groups.

C	-4.21204200	-3.17677900	-2.49203500
C	-3.08871900	-4.08282800	-2.63746800
C	-1.95112100	-3.32740800	-2.51982100
C	-2.37927800	-1.96890600	-2.28955500
N	-3.75026800	-1.89610500	-2.25291300
C	-5.57212500	-3.55065800	-2.57410500
C	-1.50069400	-0.86016000	-2.17035100
C	-1.91432600	0.48633400	-1.95587900
C	-1.02214200	1.61765200	-1.98139800
C	-1.76854100	2.71702400	-1.65198500
C	-3.12293700	2.25598100	-1.43004800
N	-3.19334300	0.89326700	-1.65208300
C	-4.19285900	3.10466500	-1.05185100
C	-5.55502800	2.71951300	-1.08921800
C	-6.68996100	3.59553300	-0.87006100
C	-7.82010000	2.83430900	-1.02920100
C	-7.37822600	1.49683000	-1.34443900
N	-6.00201800	1.44502900	-1.37188200
C	-8.23682700	0.42757200	-1.62484400
C	-7.86875000	-0.87206000	-1.98714800
C	-8.80125800	-1.92283200	-2.32746100
C	-8.05383000	-3.03827200	-2.60136000
C	-6.66340100	-2.66514400	-2.42320900
N	-6.57619100	-1.33753000	-2.07345300
Zn	-4.88204200	-0.25260800	-1.73543700
C	-3.80068800	4.46346800	-0.56664900
C	-5.88657600	-4.99789500	-2.76138500
C	-0.10178100	-1.08058300	-2.24445300
C	1.12543700	-1.13568500	-2.19497100
C	-5.48197300	-5.69938800	-3.90576500
C	-5.75778300	-7.07448100	-4.05520000
C	-6.45856900	-7.72064600	-3.02343600
C	-6.88364800	-7.04252800	-1.85888800
C	-6.58988600	-5.67743500	-1.74315800
C	-4.29065000	5.65760400	-1.13715700
C	-3.84859300	6.91060500	-0.68250200
C	-2.87716900	6.95370000	0.34413100
C	-2.35866700	5.78836800	0.93175900
C	-2.85161500	4.55580500	0.46875000
C	-0.19377900	-1.57240000	1.15238600
C	-1.42214800	-1.52152800	1.10471300
F	-6.71018000	-3.16862300	0.39751400
C	-3.76956100	-3.66749000	0.75694500
C	-3.87460800	-2.19993200	0.99881800
C	-2.80726400	-1.27674100	1.18603500
C	-3.37800600	-0.02752500	1.54153600
C	-4.78753500	-0.22405000	1.57517700
N	-5.04812000	-1.55704400	1.19327000
C	-5.84532900	0.63119000	1.99132700
C	-7.19247700	0.22840500	1.84226100
C	-8.44948000	0.88793000	2.09412900
C	-9.44228300	-0.04591400	1.79219400
C	-8.82191900	-1.25514100	1.40676700

N	-7.48031100	-1.08157600	1.41203400	H	-9.23756900	-2.87475300	0.06569800
C	-9.46771700	-2.56812600	1.09487700	H	-10.55519400	-2.49102000	1.22454700
F	-6.44477400	-2.89012700	2.66757800	H	-8.52065300	3.02166700	1.76163100
B	-6.43597900	-2.25139200	1.41941800	H	-8.15746700	2.57096900	3.43238100
C	-5.49075700	1.83502500	2.80278200	H	-9.81530100	2.37058000	2.79552300
C	-8.74644300	2.28789500	2.55007400	H	-3.15329900	2.05293000	2.09350900
C	-2.56055000	1.20857300	1.74159700	H	-2.09584600	1.48603200	0.78586400
C	-5.84643200	3.15809600	2.47406900	H	-1.74677600	1.01787400	2.45727400
C	-5.56884800	4.21714600	3.35754800	H	-6.35807000	3.33481300	1.53459300
C	-4.85156900	3.92790100	4.53707600	H	-4.62846600	4.74367900	5.22004600
C	-4.42188400	2.63186100	4.86206500	H	-4.49622400	0.56291500	4.22529000
C	-4.78386600	1.58743400	3.99425800	C	-3.56672100	2.31432400	6.10044400
H	-3.16906300	-5.15095800	-2.80548700	C	-4.31127900	1.29583300	7.00029800
H	-0.91434300	-3.64330300	-2.58468500	C	-2.22282500	1.69660000	5.63066400
H	0.03051800	1.56317700	-2.22388000	C	-6.12933900	5.64073900	3.15968300
H	-1.44283700	3.74791700	-1.58808000	C	-6.69404600	5.86867900	1.74470200
H	-6.63009200	4.64972200	-0.63901400	C	-5.05533800	6.72989800	3.40194300
H	-8.85887000	3.14704300	-0.95913200	C	-7.27811300	5.82710000	4.18708800
H	-9.30529600	0.63195900	-1.56018800	C	-5.28237300	-7.79714500	-5.32851600
H	-9.88202400	-1.80918600	-2.35626900	C	-5.64803000	-9.29608400	-5.33214600
H	-8.39547200	-4.02368300	-2.89882600	C	-5.93709400	-7.13438200	-6.56792500
H	-4.94534300	-5.16114800	-4.68675800	C	-3.74038700	-7.67244400	-5.43895700
H	-6.68382300	-8.78166500	-3.11401200	C	-7.63647000	-7.81462500	-0.76114000
H	-6.88102200	-5.11280900	-0.86328500	C	-8.01512600	-6.91718900	0.43770200
H	-5.00207100	5.58498800	-1.95615700	C	-8.93991200	-8.40750600	-1.35531700
H	-2.52697800	7.92699000	0.68309700	C	-6.74114800	-8.96878600	-0.24238600
H	-2.46403200	3.63853400	0.89579600	C	-1.27350800	5.79020600	2.02852600
H	-2.74005700	-3.92305600	0.48095100	C	-1.78024700	5.02819900	3.28076200
H	-4.45478100	-3.98556700	-0.03486600	C	-0.87278100	7.21753100	2.45201100
H	-4.05303600	-4.20926500	1.67381600	C	-0.01248000	5.05861400	1.50198400
H	-10.51488300	0.11647000	1.85880300	C	-4.37051000	8.23549000	-1.26654200
H	-9.07538000	-3.35049200	1.76133100	C	-5.42536400	8.02162400	-2.37261400

C	-3.18635600	9.03282700	-1.87147100
C	-5.02308200	9.06789800	-0.13221100
H	-3.69246300	1.04522800	7.87609800
H	-4.52771800	0.36522000	6.45681000
H	-5.26480200	1.71617500	7.35419900
H	-1.59700800	1.44985300	6.50249000
H	-1.67344200	2.40685200	4.99510500
H	-2.38667400	0.77556600	5.05349500
H	-7.10210000	6.88861400	1.67824800
H	-5.90055800	5.76456900	0.99390100
H	-7.50519000	5.16482600	1.51080000
H	-4.62577500	6.67434700	4.41203900
H	-5.51607000	7.72365200	3.29039500
H	-4.24694500	6.64117200	2.66547700
H	-6.90890000	5.70428900	5.21606800
H	-8.07418300	5.08650100	4.01751900
H	-7.71159100	6.83533200	4.08902100
H	-6.73776700	-9.44034100	-5.27969500
H	-5.18718400	-9.82178700	-4.48218200
H	-5.28430200	-9.75964200	-6.26106700
H	-5.58893400	-7.62957600	-7.48823700
H	-5.68002600	-6.06749900	-6.63228100
H	-7.03304300	-7.22064800	-6.51731100
H	-3.25185400	-8.14394200	-4.57265200
H	-3.42634700	-6.61953000	-5.47820200
H	-3.38607700	-8.17178500	-6.35464600
H	-8.67881100	-6.09595500	0.12842400
H	-7.12514500	-6.47438700	0.90831500
H	-8.54143800	-7.52090500	1.19199900
H	-9.59559700	-7.60377700	-1.72356000
H	-9.48265300	-8.97464000	-0.58257400
H	-8.72558000	-9.08607500	-2.19366600
H	-5.81270700	-8.57007800	0.19322900
H	-6.47053900	-9.66014700	-1.05382700
H	-7.27441200	-9.54030700	0.53376800
H	-0.97821600	4.99032000	4.03501000
H	-2.06821300	3.99735800	3.03621900
H	-2.65422500	5.52136600	3.72238000
H	-0.45284600	7.78054100	1.60405200
H	-0.10723700	7.16438200	3.24000400
H	-1.73579800	7.77489000	2.84724900
H	0.42547000	5.58117200	0.64129300
H	-0.25607400	4.03142400	1.20002700
H	0.75371600	5.00728100	2.29039300
H	-6.29920500	7.47257500	-1.99009400
H	-5.00781600	7.45989600	-3.22158300
H	-5.76932300	8.99841600	-2.74317800
H	-2.42155400	9.24971700	-1.11197800
H	-3.54578700	9.99000200	-2.28101700
H	-2.71085800	8.46114400	-2.68281200
H	-4.30536400	9.27776300	0.67343600
H	-5.87452500	8.52385700	0.30235600
H	-5.38543500	10.02856700	-0.53096500
C	-3.25245800	3.57120400	6.93877100
H	-4.17306100	4.03882500	7.32035000
H	-2.70241600	4.31754000	6.34587900
H	-2.62938300	3.28970400	7.80017600
F	5.72041200	-3.29183500	-0.06929100
C	8.65804500	-3.09962200	-0.02593100
C	8.28773600	-1.72247800	-0.47442000
C	9.12877600	-0.60314400	-0.65644300
C	8.38195700	0.42724100	-1.22963700
C	7.04016000	-0.08105200	-1.36833800
N	7.03423300	-1.39956100	-0.87243500

C	5.86703200	0.45714700	-1.94237500
C	4.65169600	-0.27920300	-1.92853100
C	3.32753400	0.06030200	-2.32586300
C	2.52620200	-1.07931400	-2.06819500
C	3.37537100	-2.09990700	-1.55742300
N	4.62735400	-1.60297500	-1.43892000
C	3.01914400	-3.52244200	-1.28666800
F	6.24740100	-3.20327600	-2.30942400
B	5.91472500	-2.45040700	-1.17458700
C	5.94124000	1.71853400	-2.73799500
C	2.74875000	1.33155000	-2.86336900
C	8.96011800	1.76680700	-1.58831300
C	5.73744200	1.59896000	-4.12869100
C	5.84139700	2.71410600	-4.97320900
C	6.21523200	3.94086500	-4.39245400
C	6.43536100	4.09707100	-3.01266300
C	6.25247400	2.97198700	-2.18463400
C	6.10992600	-3.29533000	2.84017400
C	7.40047500	-3.69693100	3.36867900
C	8.19244300	-2.57681000	3.36996900
C	7.39113400	-1.50296200	2.82526400
N	6.12403900	-1.95484100	2.53640400
C	5.01284600	-4.16706300	2.66541200
C	7.85218700	-0.20427800	2.58061000
C	7.11819100	0.86084200	2.04481300
C	7.62993400	2.20132700	1.88893100
C	6.59594100	2.96450700	1.40954100
C	5.45413200	2.08201600	1.26029800
N	5.79988100	0.80528600	1.64564000
C	4.17356000	2.47656200	0.79840100
C	3.05179700	1.61749100	0.73546700
C	1.70793900	2.05482700	0.41536000
C	0.89351200	0.96594900	0.54260200
C	1.72685500	-0.13200500	0.95703800
N	3.03665900	0.26945000	1.05512700
C	1.21572300	-1.43044000	1.24420600
C	1.99793900	-2.53373300	1.67523900
C	1.49244500	-3.87311100	1.85924500
C	2.56567000	-4.65150800	2.20993900
C	3.71429100	-3.76990200	2.28667600
N	3.34371000	-2.48540000	1.93844300
Zn	4.60949400	-0.88135500	1.68024500
C	3.93020300	3.91066800	0.44479600
C	5.29963100	-5.63007600	2.73897100
C	4.77000400	-6.47362000	3.72683000
C	5.03901300	-7.85619000	3.71820100
C	5.86042600	-8.36927000	2.69399200
C	6.40754900	-7.54506800	1.68979100
C	6.11465300	-6.17245500	1.72997300
C	3.39669100	4.25815300	-0.81314300
C	3.00413300	5.57276500	-1.11708300
C	3.23615600	6.56722800	-0.14392100
C	3.81071100	6.26939700	1.10642800
C	4.13172800	4.92921600	1.39180100
H	8.44855500	-3.81760900	-0.83392700
H	8.06541200	-3.40367200	0.84427100
H	9.72459200	-3.13942900	0.22928100
H	3.36375300	-3.84168500	-0.29859400
H	3.51508500	-4.16962500	-2.02810200
H	1.93234900	-3.64730000	-1.35912400
H	2.11148300	1.11316900	-3.73477700
H	3.50788500	2.05679900	-3.15768000
H	2.10327000	1.78274700	-2.09652800
H	8.69426900	2.07242600	-2.60906300

H	10.05589700	1.72226600	-1.50515300
H	8.59811900	2.55209700	-0.90900100
H	6.34717500	4.80494600	-5.04347500
H	7.64788200	-4.70187300	3.69445200
H	9.22642400	-2.48113900	3.69197200
H	8.64138200	2.51519200	2.13476900
H	6.59575000	4.02299700	1.18679000
H	1.42192400	3.06219000	0.14388900
H	-0.16859700	0.89730500	0.36585900
H	0.45709600	-4.16579700	1.71176600
H	2.58718100	-5.71709000	2.41183300
H	4.14185000	-6.04176500	4.50597900
H	6.07482100	-9.43430600	2.67485400
H	6.48653100	-5.50329800	0.95629500
H	3.25885900	3.46982700	-1.54146600
H	2.95819500	7.59413100	-0.36229600
H	4.53071600	4.66081500	2.36917800
C	4.42679200	-8.74140900	4.81973300
C	4.93012400	-8.25704800	6.20408500
C	2.88126200	-8.62075000	4.77046700
C	7.29754800	-8.07442800	0.55162500
C	6.63571000	-7.74516900	-0.81255800
C	8.68018900	-7.37435500	0.62192000
C	7.51808200	-9.59913100	0.63137400
C	2.23991600	5.86618300	-2.42636900
C	2.25170600	7.36634800	-2.80010400
C	2.80798500	5.06054600	-3.62185600
C	0.76372000	5.42850500	-2.22159000
C	4.08220900	7.34206800	2.17551100
C	3.28501700	7.00266600	3.46164800
C	5.59855300	7.35228500	2.50090600
C	3.67459100	8.75784300	1.71640800
C	5.56279900	2.64520400	-6.48390400
C	4.40647700	3.62067000	-6.82581400
C	6.83435900	3.06498000	-7.26466100
C	5.15304300	1.23039500	-6.94420800
C	6.96667700	5.44773900	-2.49325200
C	8.38459100	5.65419100	-3.08907100
C	6.05793400	6.62231100	-2.93040900
H	5.48073900	0.61965200	-4.52602800
H	6.38612000	3.04522000	-1.11051000
H	4.65848700	-7.20668800	6.38127100
H	6.02528700	-8.34373600	6.26862500
H	4.48268700	-8.86887200	7.00340800
H	2.49724000	-8.96487600	3.79812700
H	2.55666700	-7.58063300	4.91807900
H	2.42886600	-9.23749700	5.56316500
H	6.49525000	-6.66257800	-0.94208800
H	7.27195900	-8.11035000	-1.63432200
H	5.65111900	-8.23047300	-0.89084500
H	9.32289200	-7.72775100	-0.19998900
H	9.17984100	-7.59670900	1.57729200
H	8.57689900	-6.28347800	0.53389900
H	6.56382000	-10.14331600	0.56279000
H	8.01165500	-9.88365600	1.57331100
H	8.15821600	-9.92189500	-0.20294800
H	3.27714200	7.74659500	-2.91624700
H	1.73626400	7.97671800	-2.04387800
H	1.72197900	7.50521900	-3.75409700
H	2.28331400	5.36021300	-4.54171400
H	2.64883600	3.98358800	-3.49125200
H	3.88208800	5.22823500	-3.75932200
H	0.26996000	6.03334500	-1.44726600
H	0.71466400	4.37264900	-1.92001700

H	0.20153800	5.54697700	-3.16163100
H	5.81639700	8.11168200	3.26839300
H	6.18433500	7.58616300	1.59912700
H	5.93013300	6.37490600	2.88023200
H	2.59654200	8.81319200	1.50164000
H	4.22486300	9.05989700	0.81244900
H	3.90170500	9.47998800	2.51440000
H	4.65932700	4.65377400	-6.54745600
H	3.48929600	3.33737500	-6.28837800
H	4.20109200	3.59471300	-7.90760700
H	6.63824100	3.03272500	-8.34786600
H	7.66812400	2.38300900	-7.03975000
H	7.14608800	4.08651900	-7.00321500
H	4.24086500	0.89298100	-6.42964800
H	5.95123200	0.49838800	-6.75051300
H	4.95327000	1.24209200	-8.02567500
H	8.35259300	5.67824700	-4.18820900
H	9.05544900	4.83730000	-2.78306800
H	8.80685800	6.60705000	-2.73234000
H	5.07565300	6.54035200	-2.44933900
H	5.91797100	6.65455900	-4.02040600
H	6.51627600	7.57432600	-2.61921400
H	3.56102700	6.01371200	3.85397900
H	2.20458900	7.00110200	3.25434300
H	3.49169100	7.75250700	4.24147600
C	7.07242200	5.49298200	-0.95713000
H	7.76716100	4.72759900	-0.58303000
H	6.09055600	5.33953500	-0.49117100
H	7.45398900	6.47780800	-0.64829800
C	4.79951000	-10.23087900	4.66431000
H	5.88885100	-10.37745700	4.71830700
H	4.44270000	-10.63463900	3.70475600
H	4.33448700	-10.81069800	5.47533200
H	10.18491400	-0.56418900	-0.40378900
H	8.88996000	0.00354700	2.84191500

6.3. 1 for Fig. S3.

C	0.74357200	2.87356400	-0.08894100
C	-0.64654900	2.46943000	-0.01323200
C	-0.66393000	1.10117900	0.02303900
C	0.71205000	0.66656700	-0.00119700
N	1.55519700	1.75115200	-0.05975400
C	1.18639800	4.21525500	-0.17712900
C	1.11815200	-0.70065800	0.02783400
C	2.46500400	-1.15549900	0.05773300
C	2.84949200	-2.54678500	0.05940200
C	4.21876100	-2.57611800	0.08955500
C	4.67036800	-1.19828400	0.12255000
N	3.57759200	-0.34876200	0.08972300
C	6.02711500	-0.79787000	0.16139300
C	6.47164300	0.54620700	0.12894400
C	7.85940600	0.96592700	0.21789000
C	7.86697500	2.33414000	0.13964900
C	6.48874800	2.75222600	0.02280500
N	5.65552000	1.65326800	0.02404400
C	6.07013600	4.08503700	-0.07324600
C	4.75151900	4.55164600	-0.14505500
C	4.38113300	5.94033200	-0.29471100
C	3.01166700	5.98098500	-0.33768900
C	2.54510300	4.61351700	-0.19303500
N	3.62387700	3.76027700	-0.09081900
Zn	3.60457800	1.70445200	-0.00901400
C	7.06543300	-1.87000400	0.23790000
C	0.14086000	5.27938700	-0.25945600

C	0.07414300	-1.66231500	0.01259600
C	-0.91446500	-2.39167900	-0.05381000
F	-3.87546700	-7.04632900	-0.21247300
C	-1.31658500	-5.39851200	-1.09092000
C	-2.34482200	-4.40715500	-0.65553200
C	-2.13681500	-3.08396000	-0.15287700
C	-3.40871300	-2.53981000	0.15540000
C	-4.36141500	-3.53404000	-0.21510800
N	-3.66656600	-4.66411200	-0.68157200
C	-5.77363400	-3.52112400	-0.19629700
C	-6.51839300	-4.65241000	-0.57612800
C	-7.93629700	-4.85574800	-0.71503100
C	-8.09260600	-6.17337800	-1.15178600
C	-6.80741600	-6.75299700	-1.29047500
N	-5.86905600	-5.83869000	-0.94937400
C	-6.43951300	-8.12977400	-1.74767500
F	-3.98875300	-6.35297600	-2.41535100
B	-4.31447300	-6.04507400	-1.08628700
C	-6.46259300	-2.26530800	0.20291300
C	-9.05513600	-3.87716500	-0.48438800
C	-3.61183500	-1.19736900	0.79741900
C	-6.37294700	-1.13548800	-0.62837500
C	-6.94693500	0.08693300	-0.24104100
C	-7.63436800	0.12663700	0.98702300
C	-7.75045300	-0.98996800	1.83710100
C	-7.14623500	-2.19130200	1.42766000
C	-0.81887200	5.25530200	-1.28435300
C	-1.84896100	6.21407400	-1.35261900
C	-1.86911700	7.22526200	-0.37900800
C	-0.90885500	7.29692900	0.65513300
C	0.08441100	6.30816600	0.70634600
C	8.03423300	-1.99476200	-0.77684900
C	9.02147300	-2.99357800	-0.71910600
C	9.00302300	-3.87363400	0.37932100
C	8.04746700	-3.78550200	1.40934300
C	7.08346200	-2.76591400	1.32488300
H	-1.49343300	3.14532400	0.01594100
H	-1.52061700	0.43989500	0.06788900
H	2.15238600	-3.37873600	0.03288000
H	4.87000500	-3.44298900	0.08324700
H	8.70439700	0.29570500	0.33078000
H	8.72064600	3.00665800	0.17133700
H	6.85582700	4.84110300	-0.09562800
H	5.08310600	6.76703300	-0.37124800
H	2.36952100	6.84604200	-0.46176600
H	-1.56069600	-5.77662000	-2.09317300
H	-1.32282600	-6.26737700	-0.41541900
H	-0.32288800	-4.93336700	-1.08953700
H	-9.03261200	-6.67529600	-1.36528600
H	-5.82414000	-8.62925700	-0.98517500
H	-5.82243700	-8.06901100	-2.65589900
H	-7.33967300	-8.72459700	-1.94753600
H	-8.83552500	-2.89673400	-0.93025300
H	-9.23167300	-3.69855300	0.58743800
H	-9.98437300	-4.26797300	-0.92331300
H	-3.81612400	-0.41087000	0.05321400
H	-2.69747400	-0.91861900	1.34012400
H	-4.45864700	-1.20005500	1.49480800
H	-8.08828000	1.06683800	1.30010500
H	-0.76485100	4.46149200	-2.02837800
H	-2.64884600	7.98379000	-0.41036600
H	0.82990200	6.30746300	1.49840500
H	7.99627800	-1.29703500	-1.61045500
H	9.75992500	-4.65640300	0.43373700

H	6.32975600	-2.64647100	2.10011100
C	-2.90486300	6.09784600	-2.46674400
C	-3.95962800	7.22210100	-2.40420100
C	-2.20856300	6.15868900	-3.85018700
C	-3.63696900	4.73701800	-2.32327300
C	-0.99750900	8.43902200	1.68372000
C	0.12599200	8.37260500	2.73955000
C	-0.88953800	9.79876300	0.94613000
C	-2.36105100	8.36564000	2.41821600
C	8.09635700	-4.79449500	2.57080000
C	6.97713400	-4.55833400	3.60697800
C	9.46216600	-4.67862300	3.29512900
C	7.93925200	-6.22948900	2.00475400
C	10.10366200	-3.15750400	-1.80157400
C	9.97635900	-2.10980100	-2.92781200
C	9.98883200	-4.56847700	-2.43374000
C	11.50261000	-3.00274600	-1.15082500
C	-6.82321900	1.36966800	-1.08260100
C	-8.23809400	1.85744800	-1.48591500
C	-6.12682600	2.46797400	-0.23701700
C	-5.99319100	1.15656500	-2.36609700
C	-8.51704700	-0.85143800	3.16363300
C	-7.84710800	0.24544900	4.03066000
C	-9.98195200	-0.44253300	2.86173100
H	-5.81844800	-1.22299800	-1.56030900
H	-7.18915400	-3.08165000	2.05170700
H	-3.49469400	8.21305500	-2.51821500
H	-4.50690800	7.20357000	-1.44940900
H	-4.68695600	7.08903400	-3.21876100
H	-2.95633300	6.05899900	-4.65272100
H	-1.47313300	5.34969900	-3.96340000
H	-1.68537100	7.11836100	-3.97703900
H	-4.14487500	4.67319900	-1.34934500
H	-2.93508500	3.89396700	-2.39759000
H	-4.39172900	4.62800800	-3.11858400
H	1.11944000	8.43705200	2.27055700
H	0.07655700	7.43748400	3.31729400
H	0.02143200	9.21444800	3.43994100
H	0.07522200	9.87885000	0.42272900
H	-0.96464700	10.62603900	1.66946700
H	-1.69253900	9.91642900	0.20432400
H	-2.45951100	7.41024700	2.95527100
H	-3.19976000	8.45003200	1.71203900
H	-2.44088400	9.18726700	3.14743600
H	7.05591100	-5.30883200	4.40722900
H	5.98133000	-4.64877100	3.14770600
H	7.05923100	-3.56025900	4.06278000
H	10.29713800	-4.87562100	2.60726000
H	9.51516500	-5.40826900	4.11864200
H	9.59297500	-3.66925300	3.71333900
H	8.73869700	-6.46613200	1.28778100
H	6.97345300	-6.33794600	1.48849200
H	7.98245700	-6.96443200	2.82391200
H	10.07084000	-1.08646600	-2.53414800
H	9.00831500	-2.19379300	-3.44401500
H	10.77457300	-2.26799400	-3.66806300
H	10.10905900	-5.35668500	-1.67652600
H	10.76990900	-4.70346000	-3.19849700
H	9.00597400	-4.69903500	-2.91085000
H	11.66050000	-3.75040600	-0.36034800
H	11.61272600	-2.00333000	-0.70332900
H	12.28848000	-3.13392100	-1.91127800
H	-8.85766500	2.05749200	-0.59972200
H	-8.74913100	1.09902500	-2.09796600

H	-8.16289700	2.78721900	-2.07126900
H	-6.04709300	3.39553200	-0.82410900
H	-5.11289900	2.15147200	0.05105700
H	-6.69061100	2.68854800	0.68079100
H	-6.45556700	0.40528700	-3.02381100
H	-4.96993500	0.82768300	-2.12956200
H	-5.92635900	2.10411200	-2.92032100
H	-7.84426100	1.21680700	3.51545400
H	-6.80511000	-0.02513300	4.25806200
H	-8.39412900	0.36069000	4.97939000
H	-10.48216400	-1.21344400	2.25610100
H	-10.02609800	0.50783700	2.31034600
H	-10.54051300	-0.32045100	3.80286800
C	-8.53671600	-2.16473100	3.97384500
H	-7.51824800	-2.48815600	4.23621200
H	-9.02394500	-2.97533800	3.41093700
H	-9.09857700	-2.01063700	4.90649300